

New Gap Equation for A Marginal Fermi Liquid

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Assuming a phenomenological self-energy $Im\Sigma(\omega) \sim |\omega|^\beta$, ($\beta = 1$), which becomes gapped below T_c , we derived a new gap equation. The new gap equation contains the effect of the kinetic energy gain upon developing a superconducting order parameter. However, this new kinetic energy gain mechanism works only for a repulsive pairing potential leading to a s-wave state. In this case, compared to the usual potential energy gain in the superconducting state as in the BCS gap equation, the kinetic energy gain is more effective to easily achieve a high critical temperature T_c , since it is naturally Fermi energy scale. In view of the experimental evidences of the d-wave pairing state in the hole-doped copper-oxide high- T_c superconductors, we discuss the implications of our results.

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Numerous transport measurements of the high- T_c superconductors [1] indicate a very strong quasi-particle scattering rate ($1/\tau(\omega)$) up to $\sim 2000\text{cm}^{-1}$ or even higher up at the normal state, which is definitely electronic origin and is a source of most of the anomalous normal state properties such as ac/dc conductivity, NMR, Knight shift, ARPES, Raman spectra, etc [2]. This unique quasi-particle scattering rate is a finger print of a poor metallic state due to the nearness to the Mott insulator. On the other hand, this strong scattering rate is gapped below the superconducting critical temperature T_c or some higher temperature ($T^* > T_c$) for most of the underdoped compounds, as indicated by all of the experiments above mentioned. Therefore, there is a clear indication that the quasi-particle scattering rate is suppressed as a kind of gap develops in the electronic channel and this gap is closely related to the superconducting gap [3].

On the other hand, many theories have been proposed to account for such high critical temperature in the high- T_c cuprates. Certainly, it is beyond the scope of this paper to judge the level of success of these theories. One of the common ingredients of many theories is that such a strong correlation effect, as indicated in the many normal state properties, should somehow be involved in the superconducting pairing mechanism. Along this line of thinking, perhaps the Interlayer Pair Tunneling (IPT) theory, proposed early on by P.W. Anderson et. al. [4], most actively exploited this idea to the limit, such that this theory requires a spin-charge separated non-Fermi liquid ground state (called a Luttinger liquid). As a result, the c-axis normal transport is dynamically blocked (named as *confinement*) but only a momentum conserving pair tunneling process is allowed via virtual process [5]. More intuitive account of this theory is that the frustrated kinetic energy along the c-axis in the normal state, because of its Luttinger liquid ground state, is liberated in the superconducting state and this kinetic energy gain is the main source of the high critical temperature [6]. In this theory, however, there are some of the issues yet to be cleared out, such as a realization of the Luttinger liquid ground state, for example. Nevertheless, the idea of the kinetic energy gain as a source of superconducting condensation energy seems to be supported with various experiments, in particular, such as the c-axis ac conductivity and the c-axis penetration depth measurements [7].

In this paper, we take a phenomenological approach to the problem how to incorporate the kinetic energy gain upon entering a superconducting phase in the superconducting pairing mechanism, not necessarily confining in the c-axis kinetic energy. We assume that the kinetic energy frustration of the system is represented by a self-energy $Im\Sigma(\omega) \sim |\omega|^\beta$, and this self-energy becomes gapped upon developing a superconducting order parameter. We considered mainly $\beta = 1$ case since it is the most relevant case for high- T_c superconductors [1,2].

We obtained a new gap equation as a natural extension of the BCS gap equation when the condensation energy is drained not only from the potential energy but also from the kinetic energy as possibly realized with the above assumption. Oddly enough, the new gap equation shows that the kinetic energy gain works only for a repulsive pair potential and best for an isotropic s-wave state. For an attractive pair potential it works destructively and with a strong anisotropy of the order parameter the effect quickly disappears. We show some numerical results of T_c as a function of the strength of kinetic energy frustration both for a s-wave and a d-wave state in a model T_c equation. The results indicate possible competition between a s-wave and a d-wave state in high- T_c superconductors. We discuss the implications of our results in view of experiments.

We start with a usual BCS Hamiltonian.

$$H = \sum_{k,\sigma} \xi_k c_{k,\sigma}^\dagger c_{k,\sigma} + V \sum_{|k|,|k'| < \omega_D} c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger c_{k',\downarrow} c_{-k',\uparrow}, \quad (1)$$

where c^\dagger and c are the electron creation and annihilation operators, ξ_k is the electron energy including chemical potential, V is a two body pair potential. Now, assuming U(1) symmetry breaking order parameter, $\Delta = V \sum_{k'; |k'| < \omega_D} \langle c_{k',\downarrow} c_{-k',\uparrow} \rangle$, and introducing the Nambu spinor, $\psi^\dagger = (c_{k,\uparrow}^\dagger, c_{-k,\downarrow})$, we can readily obtain the free energy in the Matsubara frequency summation as follows.

$$F(\Delta, \tau) = - \left[\frac{\Delta^* \Delta}{V} + \tau \sum_k \sum_n \ln[\omega_n^2 + (\xi_k^2 + \Delta^* \Delta)] \right], \quad (2)$$

where $\tau = k_B T$ and $\omega_n = \pi \tau (2n + 1)$ is the Matsubara frequencies.

Now, minimizing the above free energy with respect to Δ , i.e., $\delta F / \delta \Delta = 0$, we obtain the usual BCS gap equation as follows.

$$\Delta = -V\tau \sum_n \sum_{k, |k| < \omega_D} \frac{\Delta}{[\omega_n^2 + E_k^2]}, \quad (3)$$

where $E_k^2 = (\xi_k^2 + \Delta^* \Delta)$.

This is a standard procedure to obtain the self-consistent mean field equation for the order parameter presumed for a given Hamiltonian. We want now to include the frustrated kinetic energy and its regaining effect in the superconducting state in the above derivation of the gap equation. We do this by including the quasi particle renormalization parameter $Z(\omega_n, \Delta)$ in the above free energy and minimizing it with respect to Δ *with special attention to the Δ dependence of $Z(\omega_n, \Delta)$* . We assume the form of a self-energy as follows, which is both experimentally [1] and theoretically motivated [8].

$$\begin{aligned} \text{Im}\Sigma(\omega) &= \alpha|\omega| \quad \text{for } 3\Delta < |\omega| < \omega_c \\ &= 0 \quad \text{for } |\omega| < 3\Delta \end{aligned} \quad (4)$$

where ω_c is an ultraviolet cutoff. For a d-wave gap, more reasonable one would be like $\text{Im}\Sigma(\omega) \sim \omega^4$ for $|\omega| < 3\Delta$. However, even in that case, we can use the above simplification because it makes no qualitative change in our main results [9]. The self-energy in the Matsubara frequency, $\Sigma(\omega_n, \Delta)$, is obtained by the spectral representation,

$$\Sigma(\omega_n, \Delta) = -\frac{1}{\pi} \left[\int_{-\omega_c}^{\omega_c} - \int_{-3|\Delta|}^{3|\Delta|} \right] \frac{\alpha|\omega'|}{i\omega_n - \omega'} d\omega' \quad (5)$$

and ω_n is accordingly renormalized.

$$\omega_n \rightarrow \tilde{\omega}_n = \omega_n Z_n = \omega_n \left[1 + \frac{\alpha}{\pi} \ln \frac{\omega_n^2 + \omega_c^2}{\omega_n^2 + (3|\Delta|)^2} \right]. \quad (6)$$

With this $\tilde{\omega}_n$ in the free energy, Eq.(2), we get

$$\begin{aligned} -\frac{\delta F}{\delta \Delta^*} &= \frac{\Delta}{V} + \tau \sum_k \sum_n \frac{\Delta}{[\omega_n^2 Z_n^2 + E_k^2]} \\ &+ \tau \sum_k \sum_n \frac{2\omega_n^2 Z_n \frac{\partial Z_n}{\partial \Delta^*}}{[\omega_n^2 Z_n^2 + E_k^2]}. \end{aligned} \quad (7)$$

Finally, we obtain the gap equation for a s-wave order parameter, $\Delta = \text{const}$.

$$\Delta = -V\tau \sum_n \sum_{k, |\xi_k| < \omega_D} \frac{[1 - \frac{\alpha}{\pi} \frac{18\omega_n^2 Z_n}{[\omega_n^2 + (3\Delta)^2]}]}{[\omega_n^2 Z_n^2 + E_k^2]} \Delta. \quad (8)$$

The T_c equation is obtained by taking $\Delta \rightarrow 0$ limit.

$$1 = -V\tau \sum_n \sum_{k, |\xi_k| < \omega_D} \frac{[1 - \frac{\alpha}{\pi} 18Z_n^{(0)}]}{[\omega_n^2 Z_n^{(0)2} + \xi_k^2]}, \quad (9)$$

where $Z_n^{(0)} = Z_n(\Delta = 0)$. This is our main result and now let's analyze the above gap equation. The term, $\frac{\alpha}{\pi} 18Z_n^{(0)}$, in the numerator in the right-hand side of Eq. (9) is the new term originating from the kinetic energy gain; otherwise, Eq. (9) is a simple BCS T_c equation with just an ordinary self-energy correction, Z_n , in the denominator. As well known, if not the new term, the above equation can have a solution only for an attractive interaction (i.e. $V < 0$). However, with the new term, it can have a solution even with a purely repulsive interaction (i.e. $V > 0$) since $\frac{\alpha}{\pi} 18 \sim 2.9$ with $\alpha \sim 0.5$ (which is a reasonable value for the high- T_c cuprates [1]) and $Z_n > 1$ always. What if $V < 0$ then? It is a disaster. The new kinetic energy gain term works only for a repulsive pair potential but it works destructively for an attractive pair potential. Therefore I think that the newly found self-energy derived term contains some more physics than the kinetic energy gain, as discussed later.

In the case of d-wave order parameter, H_{int} and $\Delta(k)$ is defined as follows.

$$\begin{aligned} H_{int} &= \sum_{k, k'} V(k, k') c_{k\downarrow}^\dagger c_{-k\uparrow}^\dagger c_{k'\uparrow} c_{-k'\downarrow}, \\ \Delta(k) &= \langle \sum_{k'} V(k, k') c_{k'\uparrow} c_{-k'\downarrow} \rangle. \end{aligned} \quad (10)$$

Here, $V(k, k')$ is a positive definite pair potential in momentum space and $\Delta(k)$ is a sign-changing order parameter of d-wave symmetry. The gap equation can be derived similarly by taking a variation of the free energy, F_{D-wave} , with respect to $\Delta(k)$; it is slightly more involved than the s-wave case since the order parameter has a structure. The result is written as,

$$\begin{aligned} \Delta(k) &= -\tau \sum_n \sum_{k'} \frac{V(k, k') \Delta(k')}{[\omega_n^2 Z_n^2 + E_{k'}^2]} \\ &+ \tau \sum_n \sum_{k'} \frac{V(k, k') \frac{\alpha}{\pi} \frac{18\omega_n^2 Z_n}{[\omega_n^2 + (3\Delta_{max})^2]}}{[\omega_n^2 Z_n^2 + E_{k'}^2]} \Delta_{max} \frac{\delta \Delta_{max}}{\delta \Delta(k')}. \end{aligned} \quad (11)$$

Note that the second term contains now $\frac{\delta \Delta_{max}}{\delta \Delta(k')}$, which has just measure zero since it equals $\delta_{k', k'} \text{sgn}(\Delta(k'))$; it would be just 1 in the s-wave case. Therefore, the new kinetic energy gain term practically has no contribution in the d-wave gap equation; more generally, its effect quickly vanishes for any anisotropic gap $\Delta(k)$ unless Δ_{max} has a finite support in k -space [10]. Now in order to gain some more insight about the newly found term, we recall the self-consistency definition of the order parameter, $\Delta(k) = \langle \sum_{k'} V(k, k') c_{k'\downarrow} c_{-k'\uparrow} \rangle$. At first sight, the second term in Eq. (11) appears to be a redundant term. Although it is not rigorously proved here, this extra term doesn't ruin the self consistency but actually completes it. We note that the right-hand side of Eq. (11) is the pair susceptibility (a kind of response function) with respect to the U(1) symmetry breaking source, $\Delta(k)$. The first term in the right-hand side of Eq. (11) is the usual pair susceptibility including the self-energy correction, $Z(\omega_n, \Delta)$. It is well known that a vertex correction is necessary whenever a self-energy correction is included in order to satisfy some continuity equation (or underlying symmetry) for any response function. Therefore, we can consider the self-energy derived second term as a corresponding vertex correction – it indeed looks like so. And in this sense, the new extra term should contain not only the kinetic energy gain effect but also some other complicate effect (general backflow).

Now let us show some numerical results of a model T_c equation. All calculations are performed in two dimensional momentum space assuming a circular Fermi surface for simplicity of calculations. In Fig.(1) we show T_c as a function of α , the strength of inelastic scattering, both for s-wave and d-wave states with different values

of the coupling constant, λ , ($\lambda = VN(0)$, $N(0)$ is the density of states at Fermi level). For all calculations, the ultraviolet cutoff scale ω_c is taken to be $0.5eV$ and the BCS potential cutoff ω_D to be $0.5eV$ since the source of the pairing interactions must be an electronic origin. This choice of parameters is mainly for exemplary purpose, though. For a s-wave state, the results of $\lambda = 0.1$ and 0.2 are shown – extremely weak repulsive potentials, otherwise we would get much too high T_c . The message is clear; we can easily achieve several hundreds K of T_c with a very weak repulsive interaction and it increases with more kinetic energy frustration (i.e., with a larger value of α) as expected from the Tc equation, Eq. (9). For a comparison, we show a d-wave case (solid square). For a d-wave state, we drop the second term in the gap equation, Eq. (11), as explained above and the Tc equation is obtained by taking $\Delta(k) \rightarrow 0$ limit. For simplicity of numerical calculations, we assume $V(k, k') = V|\sin(\phi - \phi')|$ and $\Delta(k) = \Delta_{max}\cos(2\phi)$ in two dimensional momentum space with a circular Fermi surface, and ϕ is an angle along the Fermi surface. With $\omega_c = 0.5eV$ and $\omega_D = 0.5eV$ as in the s-wave case, we need $\lambda = 1.5$ (an order of magnitude stronger interaction) in order to get a comparable T_c ($\sim 100K$) for $\alpha \sim 0.4 - 0.6$. This value of α is the experimental value near optimal doping with $T_c \sim 90K$ in YBCO [1]. T_c quickly decreases with α increasing since now α just enters the ordinary pair-breaking self-energy correction in contrast to the s-wave case. The results show that if the ground state of the system is a marginal Fermi liquid (or even when only some part of Fermi surface is marginal Fermi liquid like) there is a possible competition between a s-wave state and a d-wave state for the experimentally relevant range of α , provided there is a weak repulsive interaction in the s-wave channel [11].

Some remarks and speculations are in order. First, in this paper we considered only $\beta = 1$ case ($Im\Sigma(\omega) \sim |\omega|^\beta$). we can easily extend our analysis to the other power. In general, $\delta Z_n(\Delta)/\delta\Delta \sim \Delta^\beta$. As a result, if the system is a Fermi liquid ($\beta = 2$), the kinetic energy gain term simply drops out of the Tc equation [9]. On the other hand, if β is any power less than 1, the kinetic energy gain term becomes singular as $\Delta \rightarrow 0$ and the gap equation becomes a non-linear equation. In this sense, $\beta = 1$ case is marginal not only for breaking Fermi liquid [2] but also for the superconducting instability. Second, it is straightforward to extend our formalism to include c-axis dynamics by introducing an anisotropy in ξ_k and a cylindrical shape of order parameter $\Delta(k)$. The whole formalism goes as the same as in two dimension. There is no kinetic energy gain effect for a d-wave order parameter in regard to enhancing T_c as the system undergoes from the incoherent state to the coherent state. The inter-layer pair tunneling mechanism by Anderson et. al. [4,5] is certainly a different approach from ours. It is not clear how to reconcile two approaches at present. Third, as

a pure speculation and viewing our numerical results, it may be that the s-wave instability and the d-wave instability closely compete in the marginal Fermi liquid state depending on the potential strength of the s-wave and d-wave channels. Then our results might be relevant to the electron-doped high- T_c compound [12].

In conclusion, assuming a phenomenological self-energy, $Im\Sigma(\omega) \sim |\omega|^\beta$, ($\beta = 1$), we derived a new gap equation which includes the kinetic energy gain effect. It is argued that the new gap equation is a natural extension of the BCS gap equation with a consistent vertex correction when the self-energy is a functional of the gap function. For the corresponding Tc equation, it is also shown that the new kinetic energy gain term becomes relevant only when $\beta \leq 1$, and $\beta = 1$ is the marginal case. When $\beta = 1$, the new Tc equation can provide surprisingly high critical temperature for the case of an isotropic s-wave order parameter with a pure repulsive potential. For the d-wave case, the new kinetic-energy gain term drops from the Tc equation because of the anisotropy of the order parameter. Numerical results indicate that there can be a competition between the s-wave and d-wave instabilities in a marginal Fermi liquid state depending on the strength of pair potential in s-wave and d-wave channels. In view of the facts that there is a substantial strength of repulsive interaction in s-wave channel besides the interaction in d-wave channel in the Hubbard or t-J model and its relevance to high- T_c superconductors, our results may have some relevance to the electron-doped high- T_c compound. Considering the unexpected behaviors of the new gap equation, it is desirable to have further investigations of it.

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⁹ The approximate treatment of $Im\Sigma(\omega)$ for $|\omega| < 3\Delta$ is irrelevant for the T_c equation as far as $\gamma > 1$ in $Im\Sigma(\omega) \sim |\omega|^\gamma$ for $|\omega| < 3\Delta$ since the effect of any higher power term ($\gamma > 1$) drops out in the T_c equation as taking $\Delta \rightarrow 0$ limit. However, it makes a difference for the determination of gap value $\Delta(T)$ from the gap equation.

¹⁰ $\frac{\delta\Delta_{max}}{\delta\Delta(k')}$ in Eq.(11) is correct only for the T_c equation because of the same reason as explained in [9]. In general, we need a functional derivative, $\frac{\delta Z_p(\Delta(k))}{\delta\Delta(k')}$. Then $\Delta(k) < \Delta_{max}$ would contribute to the detailed shape of $Im\Sigma(\omega)$ for $|\omega| < 3\Delta_{max}$ and quite generally we can guess $Im\Sigma(\omega) \sim |\omega|^\gamma$ with $\gamma > 1$ for any anisotropic order parameter. Then as argued in [9], only Δ_{max} part matters for the T_c equation. A possible exception is the case when Δ_{max} spans a finite region in momentum space.

¹¹ Some might argue that the s-wave channel should be attractive in real metals if the phonon mediated interaction and the retardation are taken into account. The retardation is not compulsory, though. If the system can lower the energy by developing superconducting order parameter without taking advantage of the retardation, it will do so.

¹² Most of experiments on the electron-doped compound (NCCO) indicate a s-wave state; however, the normal state properties of it show more Fermi liquid like behaviors (private communication with Jae H. Kim).

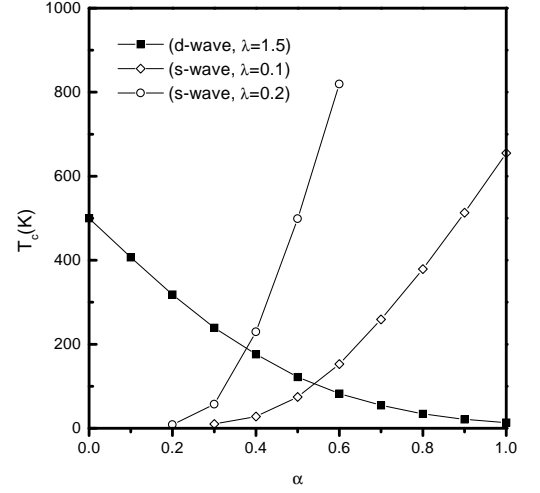


Fig.1
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FIG. 1. T_c vs α ($Im\Sigma(\omega) = \alpha|\omega|$). For all data, $\omega_D = 0.5eV$ and $\omega_c = 0.5eV$; solid square (d-wave, $\lambda = 1.5$), open circle (s-wave, $\lambda = 0.2$), and open diamond (s-wave, $\lambda = 0.1$).